Hexane, 1-methoxy-

Other names:	Ether, hexyl methyl
	Hexyl methyl ether
	Methyl hexyl ether
	1-Methoxyhexane
Inchi:	InChI=1S/C7H16O/c1-3-4-5-6-7-8-2/h3-7H2,1-2H3
InchiKey:	ICBJCVRQDSQPGI-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCCCOC
Mol. weight [g/mol]:	116.20
CAS:	4747-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-96.94	kJ/mol	Joback Method
hf	-320.03	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	42.10	kJ/mol	NIST Webbook
ie	9.48	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	2.213		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	818.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	822.80		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	823.00		NIST Webbook
ripol	940.00		NIST Webbook
ripol	960.00		NIST Webbook
ripol	924.00		NIST Webbook
ripol	941.00		NIST Webbook
tb	399.20	K	NIST Webbook
tc	546.34	K	Joback Method
tf	190.88	K	Joback Method

vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.44	J/mol×K	381.98	Joback Method
cpg	229.92	J/mol×K	409.37	Joback Method
cpg	241.06	J/mol×K	436.77	Joback Method
cpg	251.87	J/mol×K	464.16	Joback Method
cpg	262.35	J/mol×K	491.56	Joback Method
cpg	272.49	J/mol×K	518.95	Joback Method
cpg	282.30	J/mol×K	546.34	Joback Method
dvisc	0.0039006	Pa×s	190.88	Joback Method
dvisc	0.0017217	Pa×s	222.73	Joback Method
dvisc	0.0009325	Pa×s	254.58	Joback Method
dvisc	0.0005789	Pa×s	286.43	Joback Method
dvisc	0.0003953	Pa×s	318.28	Joback Method
dvisc	0.0002894	Pa×s	350.13	Joback Method
dvisc	0.0002231	Pa×s	381.98	Joback Method
hvapt	34.93	kJ/mol	399.20	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4747073&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume